Supplementary Material

High-power ^{1}H composite pulse decoupling provides artifact free Exchange-mediated Saturation Transfer (EST) experiments

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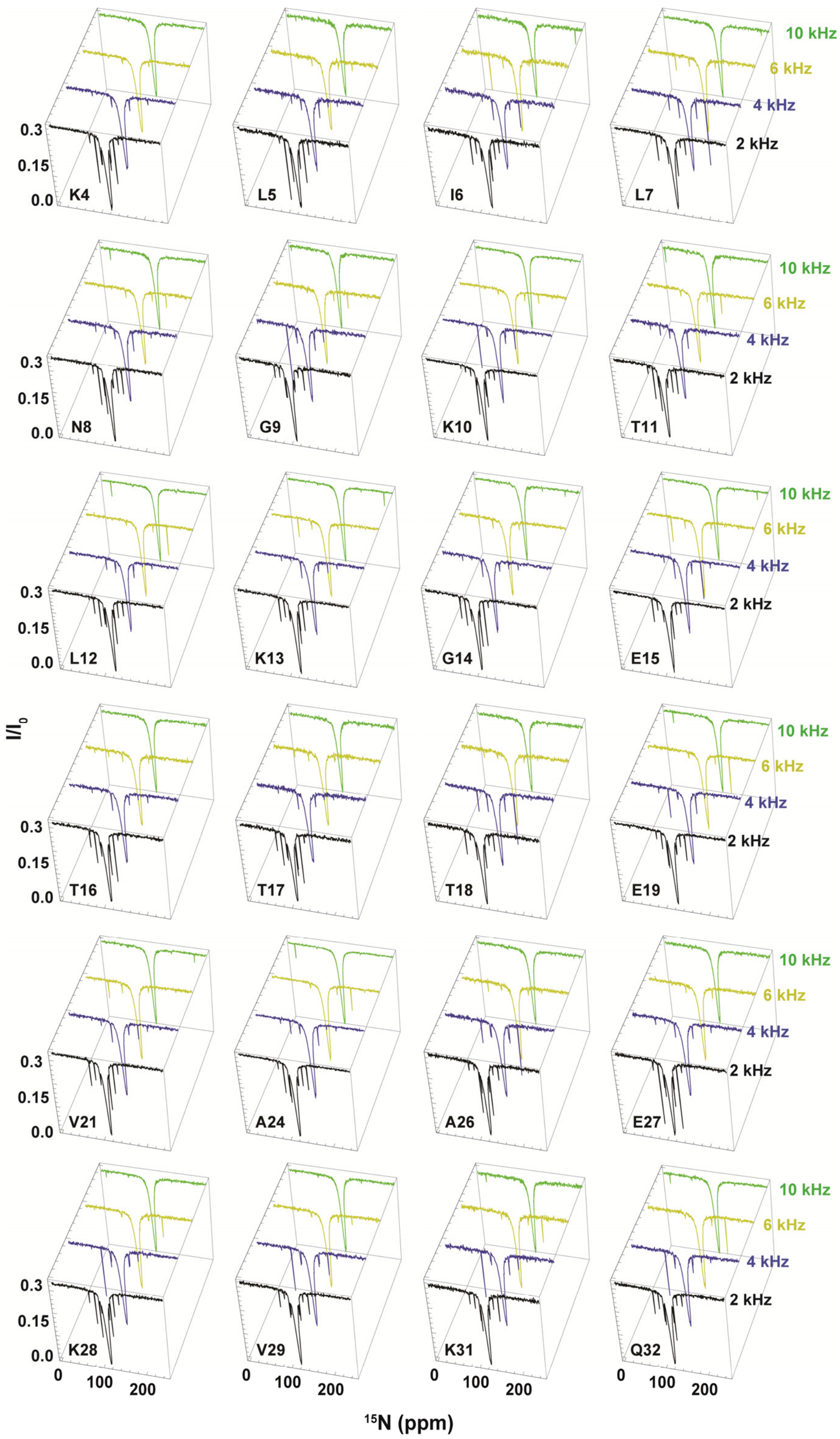
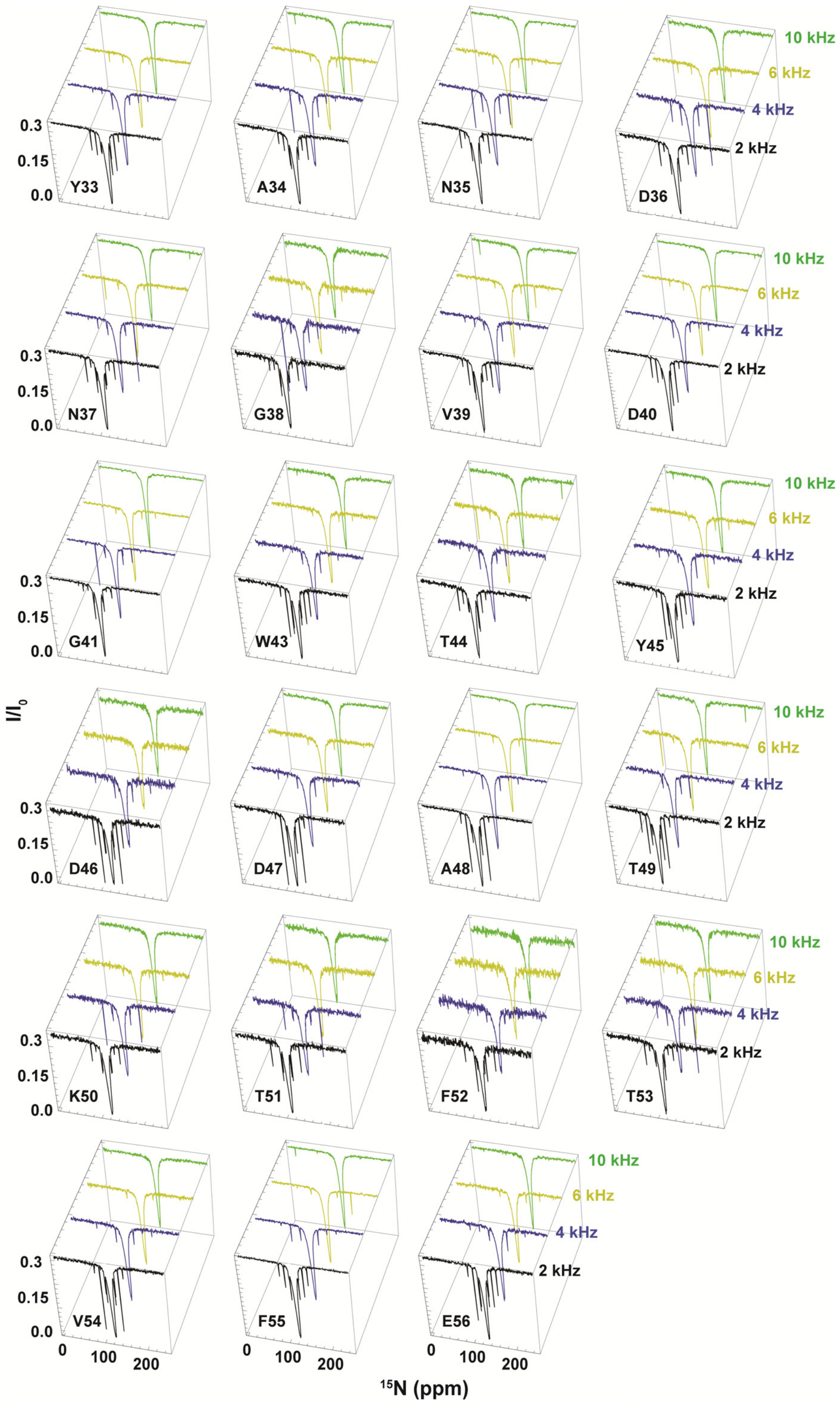
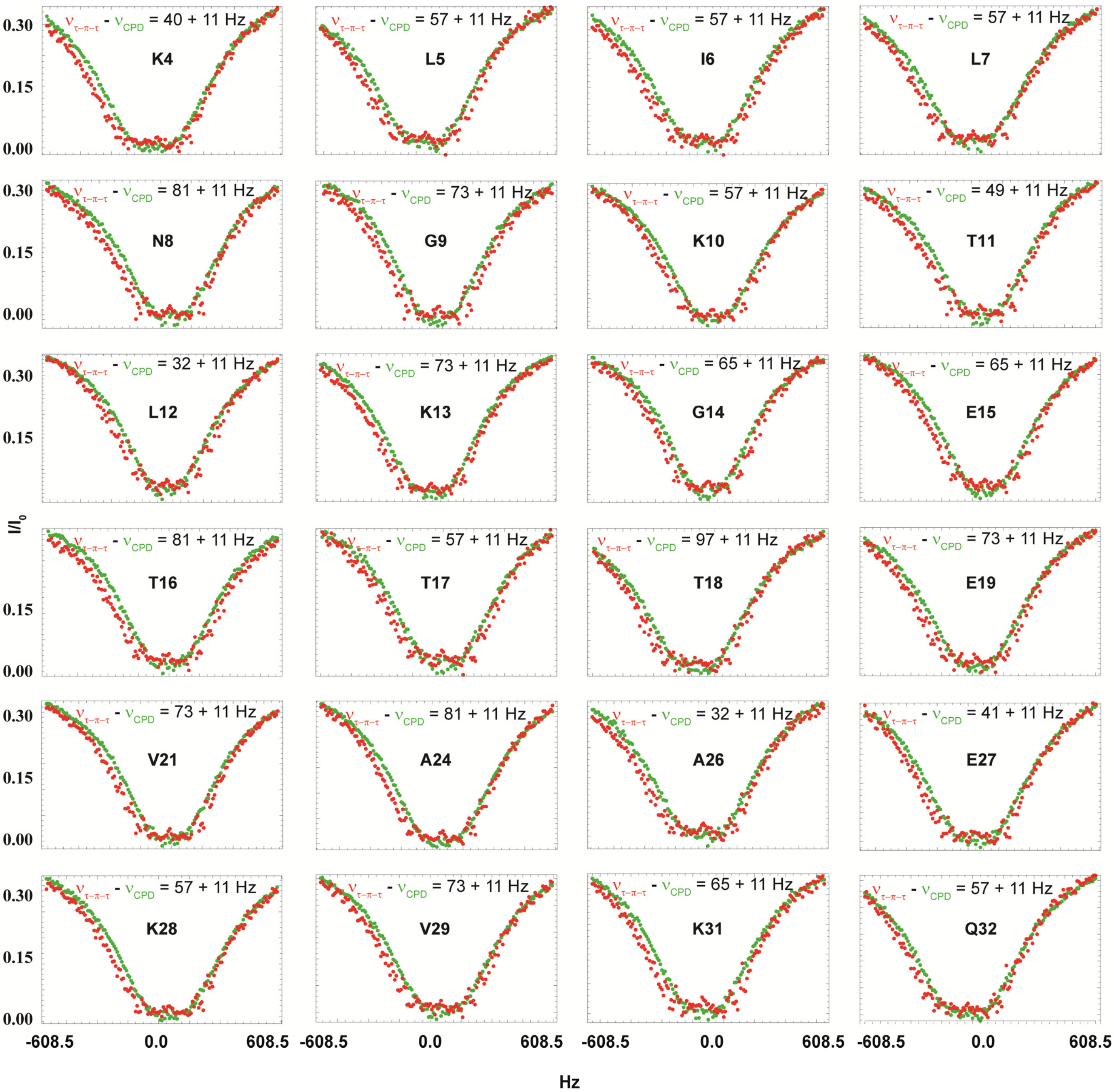
Supplementary figures

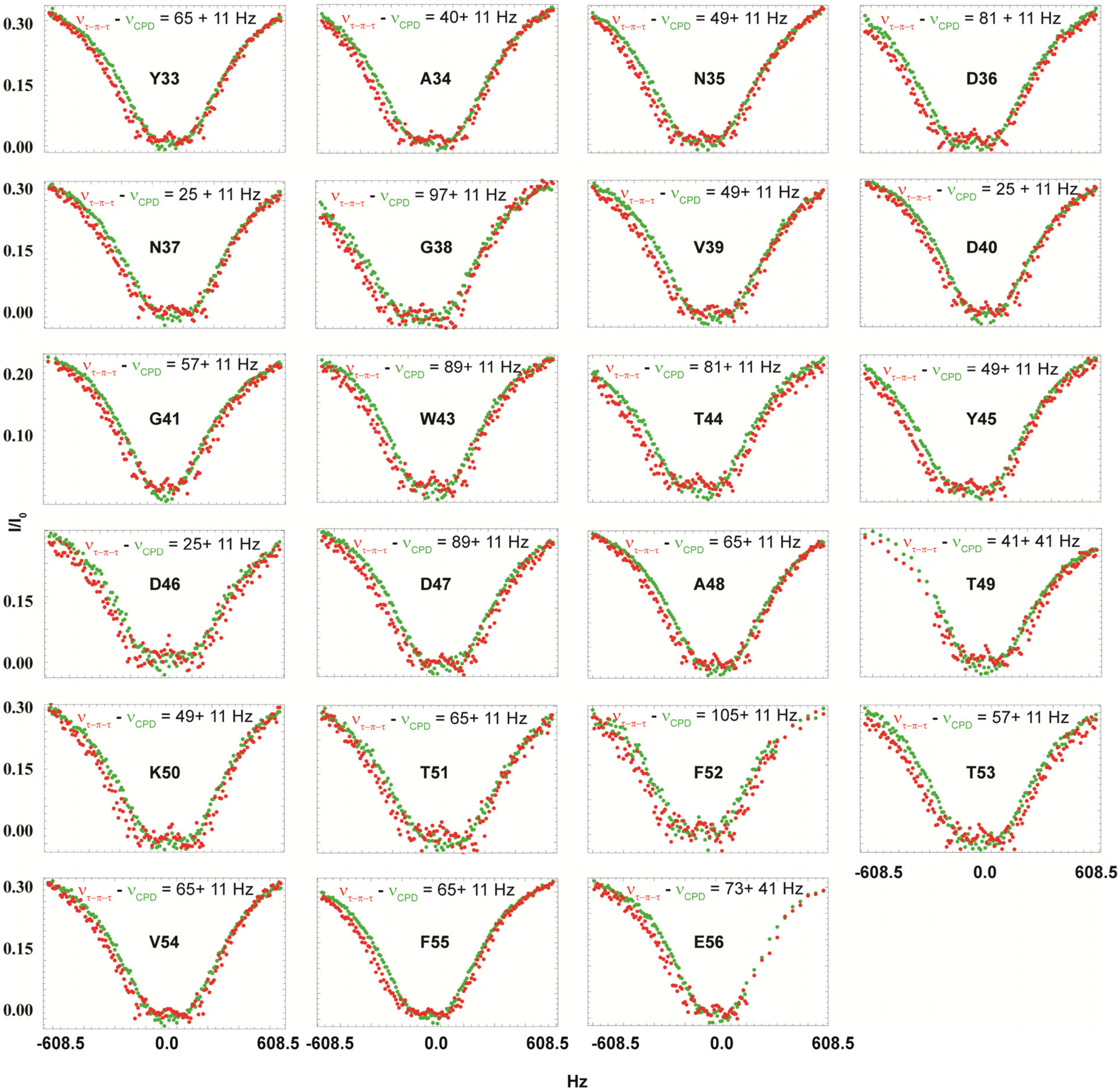




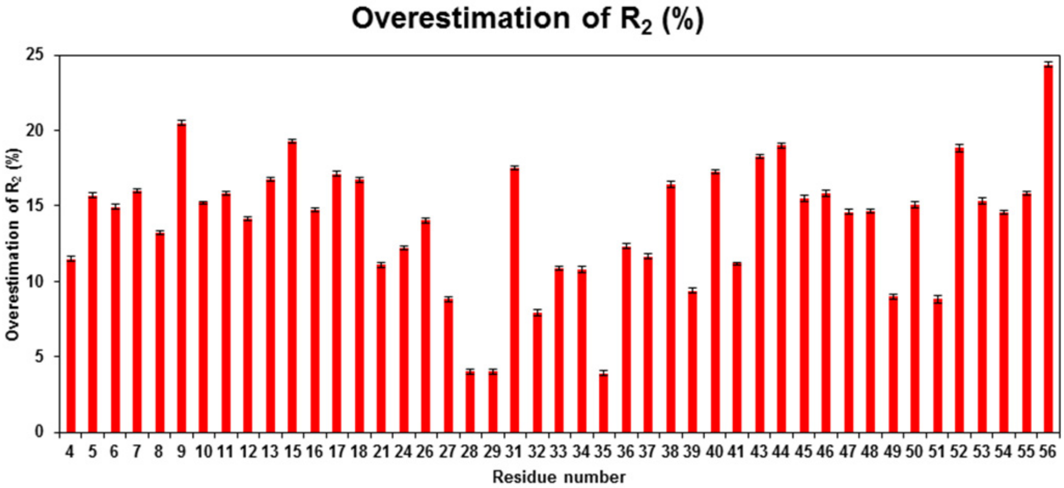
Supplementary Fig. S1. The effect of varying the ^{1}H CPD field strength on EST profiles for all residues of GB1. The EST profiles were recorded with a ^{1}H CPD field strength amplitude of 2 (black), 4 (blue), 6 (yellow) and 10 kHz (green). An increase in ^{1}H CPD field strength suppresses the magnitude of the decoupling sidebands and moves them further from the on-resonance intensity attenuation dip. All the experimental parameters are as described in Fig. 1.



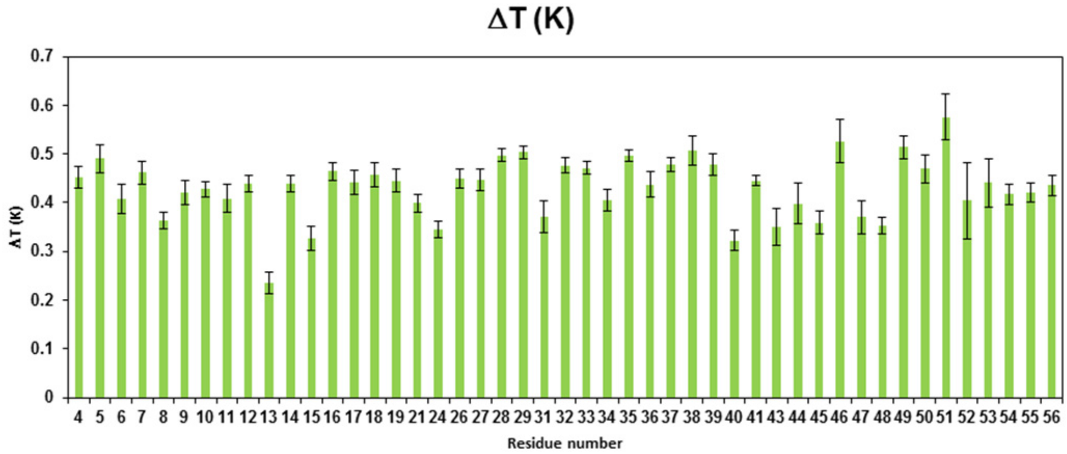
ντ-π-τ - νCPD = 40 + 11 Hz
K4
ντ-π-τ - νCPD = 57 + 11 Hz
L5
ντ-π-τ - νCPD = 57 + 11 Hz
I6
ντ-π-τ - νCPD = 57 + 11 Hz
L7
ντ-π-τ - νCPD = 81 + 11 Hz
N8
ντ-π-τ - νCPD = 73 + 11 Hz
G9
ντ-π-τ - νCPD = 57 + 11 Hz
K10
ντ-π-τ - νCPD = 49 + 11 Hz
T11
ντ-π-τ - νCPD = 32 + 11 Hz
L12
ντ-π-τ - νCPD = 73 + 11 Hz
K13
ντ-π-τ - νCPD = 65 + 11 Hz
G14
ντ-π-τ - νCPD = 65 + 11 Hz
E15
ντ-π-τ - νCPD = 81 + 11 Hz
T16
ντ-π-τ - νCPD = 57 + 11 Hz
T17
ντ-π-τ - νCPD = 97 + 11 Hz
T18
ντ-π-τ - νCPD = 73 + 11 Hz
E19
ντ-π-τ - νCPD = 73 + 11 Hz
V21
ντ-π-τ - νCPD = 81 + 11 Hz
A24
ντ-π-τ - νCPD = 32 + 11 Hz
A26
ντ-π-τ - νCPD = 41 + 11 Hz
E27
ντ-π-τ - νCPD = 57 + 11 Hz
K28
ντ-π-τ - νCPD = 73 + 11 Hz
V29
ντ-π-τ - νCPD = 65 + 11 Hz
K31
ντ-π-τ - νCPD = 57 + 11 Hz
Q32
0.30
0.15
0.00
I/I0
-608.5
0.0
608.5
Hz



Supplementary Fig. S2. The increased width of EST profiles for ^{1}H decoupling consisting of the τ–π–τ scheme (red circles) compared to the CPD scheme (green circles) for all residues of GB1. On an average the EST profile with τ–π–τ scheme is 62 ± 19 Hz wider compared to the CPD scheme. The center of the x-axis is aligned to the respective peak positions in the ^{15}N (Hz) dimension for each profile. All the experimental parameters are the same as described in Fig. 1. The region outside 100 ppm to 136 ppm along ^{15}N dimension is sampled at offsets separated by 40 Hz, resulting in fewer data-points in the intensity attenuation profiles at the most upfield resonance T49 and most downfield peak E56 and is also reflected in the errorbars calculated using the equation described in Fig. 2.



Supplementary Fig. S3: The additional width of the EST profile arising from incomplete decoupling using the $\tau{-}\pi{-}\tau$ ^{1}H decoupling scheme manifests in overestimation of the transverse relaxation rate (R_2) for backbone ^{15}N nuclei in all residues of GB1. EST profiles measured by both $\tau{-}\pi{-}\tau$ and CPD were individually fit to the Bloch-McConnell equation without chemical exchange [1]. The $\tau{-}\pi{-}\tau$ scheme compared to CPD at 10 kHz rendered R_2 values that were greater on average introducing a systematic error of 14 ± 4% for all residues of GB1. The errors in individual R_2 values were calculated from the covariance matrix method.



Supplementary Fig. S4: The amount of sample heating during the application of a ^{1}H decoupling field strength of 10 kHz was determined by calculating the change in temperature between amide proton frequencies between the reference EST spectrum and EST experiment with decoupling. Amide proton temperature coefficients of GB1 were used to determine the change in temperature. For all observable GB1 resonances the calculated increase of temperature was less than 0.6 K. Error bars were determined from the ratio between linewidth and signal to noise ratio of a given resonance.

Reference

[1] M.G. Carneiro, J.G. Reddy, C. Griesinger, D. Lee, Speeding-up exchange-mediated saturation transfer experiments by Fourier transform, J. Biomol. NMR 63 (2015) 237-244.